# Raytracing simulations for Mirror Electron Microscopy


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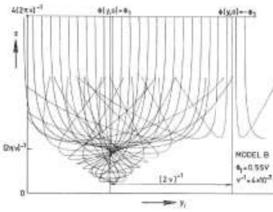
## SOLVE THE RIGHT EQUATIONS

Cosine sample potential: $V(y,0) = V_1 \cos(2\pi n v y)$

$V(y,z) = V_1 \cos(2\pi n v y)\,.\,e^{-2\pi n v z}$

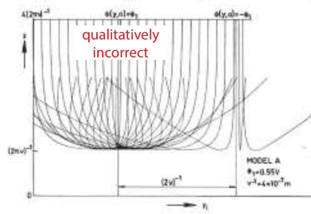
$$-e\frac{\partial V(x,y,z,)}{\partial x} = m\frac{dx^2}{dt^2}\;;\; -e\frac{\partial V(x,y,z,)}{\partial y} = m\frac{dy^2}{dt^2}\;;\; -e\frac{\partial V(x,y,z,)}{\partial z} = m\frac{dz^2}{dt^2}$$




Not good!
But often
assumed

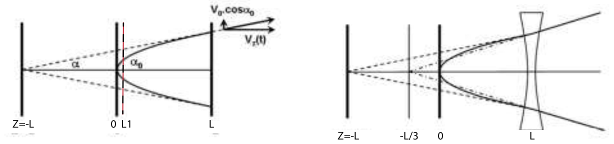
Common approximation:

$$-e\frac{\partial V(x,y,z,)}{\partial x} = m\frac{dx^2}{dt^2}\;;\; -e\frac{\partial V(x,y,z,)}{\partial y} = m\frac{dy^2}{dt^2}\;;\; -e\varepsilon = m\frac{dz^2}{dt^2}$$




A. Bok, A Mirror Electron Microscope, Doctoral Thesis, Delft, 1968
Solved on an analog computer (digital computer too limited)

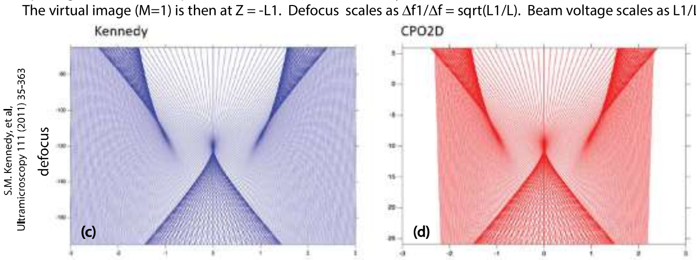
## DON'T DO TOO MUCH

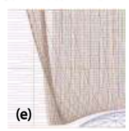



(a) Uniform field only
Virtual image at Z = -L , M = 1

(b) Uniform field with diverging objective lens opening
Virtual image at Z = -L/3 , M = 2/3

No need to ray-trace from Z = L to Z = 0 and back to L (a), or to include the diverging action of the objective opening (b). The purely parabolic part of the trajectories, or the divergence at the objective lens opening, contain no sample information. Instead, we can ray-trace from/to Z = L1<< L (see (a)).
The virtual image (M=1) is then at Z = -L1. Defocus scales as $\Delta f1/\Delta f$ = sqrt(L1/L). Beam voltage scales as L1/L.

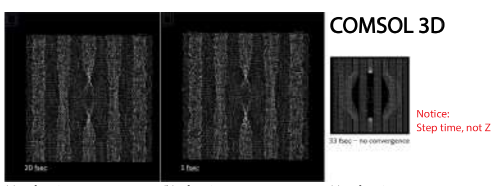


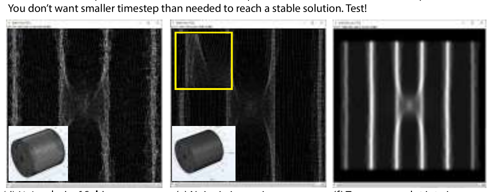

(c) simulation for a hemispherical cap, using the full geometry in (b) , including divergence at the objective lens opening. L = 2 mm.
(d) 2D CPO simulation using L1 = 10 $\mu$m.
Defocus is scaled according to $\Delta f1/\Delta f$ = sqrt(L1/L) .
The results are virtually identical.
(e) sample geometry and raytraces

We have used two software packages : CPO (electronoptics.com, boundary element method) and COMSOL (www.comsol.com, finite element method).
Good results were obtained with both programs. COMSOL has faster execution ( 2 msec/ray, vs 19 seconds/ray for CPO). CPO is a single thread process only.
We trace electrons from Z = L1, to the sample at Z = 0, and back to L1 (reflection geometry). Electrons start parallel to the optical axis.
Near the sample they undergo deflections due to sample topography and/or lateral potential gradients. Back at Z = L1, (x,y) and (dx/dz, dy/dz) are recorded for each trajectory.
Rays are then extrapolated to Z = -L1, the location of the in-focus virtual image at M=1, or to a plane at defocus $\Delta$f1, i.e. Z = -L1+$\Delta$f1. By doing this as a function of $\Delta$f1,
we obtain a defocus series . We can extrapolate to different planes in the X and Y directions, corresponding to two-fold astigmatism.

### COMSOL 3D



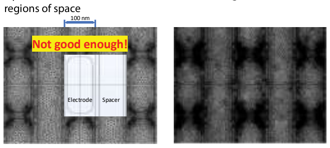

(a) 20 fsec time step (b) 1 fsec time step (c) 33 fsec time step
You don't want smaller timestep than needed to reach a stable solution. Test!



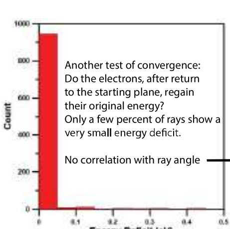
(d) Noise=lack of field convergence
Optimize 3D mesh in different regions of space

(e) Noise in image is gone: well-converged fields

(f) Turn pepperplot into image: each dot in (e) is convoluted with a Gaussian kernel - quick & easy

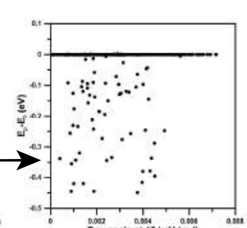



(g) extremely fine mesh may be required near the cathode (strong field gradients and/or topography)
>12M mesh elements total



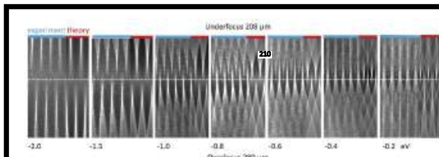

Another test of convergence:
Do the electrons, after return to the starting plane, regain their original energy?
Only a few percent of rays show a very small energy deficit.

No correlation with ray angle

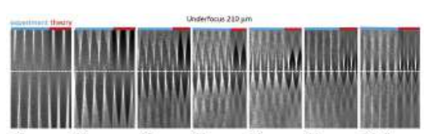



## MAKE SURE IT CONVERGES

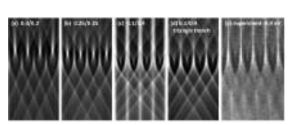
### CPO



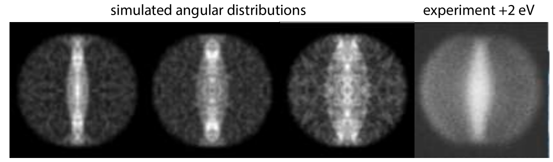

Through-focus image series of Si lines.
Repeat spacing 500 nm
Nominal line width 250 nm
Nominal line depth 250 nm
Theoretical results are for $\Delta E$ = 0 eV .




Same as above, but now the theoretical results are convoluted with the actual energy distribution of the Cold Field Emission gun.



Optimizing agreement with experiment.
(a) 300 nm line, 200 nm space
(b) 250 nm line, 250 nm space
(c) 100 nm line, 400 nm space
(d) 100 nm line, 400 nm wide triangular space.
(e) experiment at -0.4 eV




In CPO secondary electrons can be generated when and where the primary electron hits the sample.
This allows us to study the angular distribution (diffraction plane) in the LEEM regime.
The experimental result at +2 eV for a metal grating sample is shown on the right.
Simulations for different geometries are also shown for 250 nm lines and spaces.
Left to right: 350, 300, and 250 high lines.
**Notice: Ewald sphere is not round!**

## COMPARE WITH EXPERIMENT


Questions?
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